GENERAL METHOD FOR COMPARTMENTAL MODELLING OF REACTORS USING TRACER EXPERIMENTS AND CFD SIMULATIONS

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Abstract

The modelling of chemical reactors is necessary to understand and predict their behavior. Recently an approach named "compartmental modelling", based on the description of the reactor by a complex network of both structural and functional compartments derived from tracer experiments, technical information about the studied process and from CFD simulations was developed for some specific examples using very different rules from one author to another. The aim of this study is to develop a theoretical general methodology for compartmental modeling taking into account hydrodynamics, heat and mass transfer and chemical kinetics.

Keywords

MODELLING, COMPARTMENT, COMPUTATIONAL FLUID DYNAMICS, TRACING.

Introduction

Modelling of chemical reactors can be based on three approaches corresponding to three levels of description:

(i) The systemic method based on an interconnected network of maximum a dozen elementary reactors (plug flow, perfect mixing reactor, dead volume…) representative of the main hydrodynamic behavior. It is a global approach that has been extensively used in the past and still remains useful for rapid prediction. However, when local phenomena are involved, it becomes unsatisfactory and has only limited predictability, especially for scale-up.

(ii) The reactive computational fluid dynamics (CFD) method based on the resolution of the Navier-Stokes equations in a large number of computing cells (typically hundreds of thousands of cells): Despite its power, this approach still remains difficult to handle when it is desired to simulate complex hydrodynamics, heat and mass transfer and chemical reactions all together because it requires significant computational time. Moreover the overabundance of information is sometimes a disadvantage.

(iii) An intermediate approach, namely the "compartmental modeling" relies upon the description of the reactor by a structural and functional subdivision of around a few hundred compartments. These compartments are created using information deduced from tracer experiments, technical information about the studied process and CFD flow simulation.

Previous studies show that, when they are properly set-up, compartmental models give similar predictions in terms of chemical reactions as those of CFD simulations with lower calculation time with the advantage to give a simpler representation of the reactor behavior. Every existing study of the literature is devoted to a specific reactor with a given approach and cannot be straightforwardly transposed to another reactor. The aim of the present study is to analyze the existing methods and to propose a general approach of the compartmental modeling methodology.

State of art of existing methods

Compartmental modelling consists in dividing the reactor volume into smaller volumes named compartments. All of them have two important characteristics: (i) a spatial localization (ii) a physical meaningful function. Then, exchanges fluxes must be defined by convective and/or turbulent way. Figure 1 illustrates this concept. Different ways exist in order to determine the network of compartments. (Rigopoulos and Jones, 2003) have studied a bubble column. Their network is composed of three vertical tanks in series (zone rich in gas, zone poor in gas and down flow). The number of tanks is determined by fitting numerical and experimental residence time distributions (RTD). Convective fluxes between compartments represent the main recirculation loops whereas turbulent fluxes are used in order to describe gas dispersion in the riser. A phenomenological

model of interfacial mass transfer is coupled with simple chemical reactions.

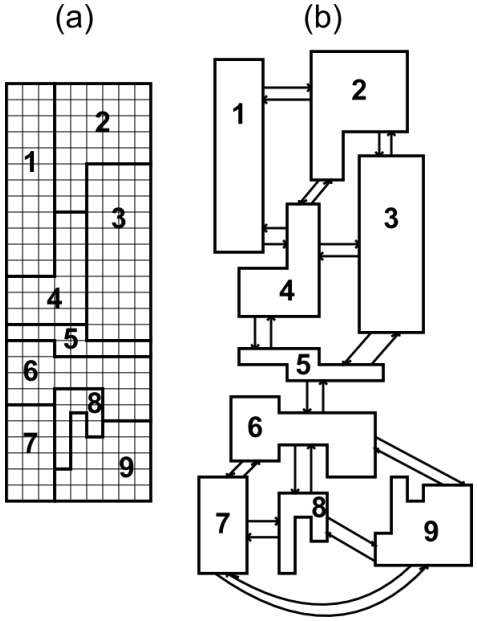

Figure 1 : Schematic main concept of compartmental modelling. (a) Creation of compartments from CFD grid. (b) Definition of exchanges fluxes.

(Guha et al., 2006) have studied a mechanically agitated reactor in order to predict the effect of mixing on the performance of the reactor. Different kinetics have been tested. The effects of mixing becomes pronounced when the time scales of some of the reactions are small compared to the time scale of mixing, then the cutting criteria is obtained with consistent time scales between reaction and hydrodynamics. (Le Moullec et al., 2010) have studied a biological reactor of wastewater treatment. The network is based on several vertical slices, each slice is composed of three zones (a high gas concentration zone, a low velocity zone and a recirculation zone). The number of slices was derived by fitting numerical and experimental RTDs. The network scheme gives a comprehensive illustration of the reactor behavior. (Delafosse et al., 2014) have studied mixing inside a mechanically agitated batch column. Only hydrodynamics is modelled with comparison of mixing time curve obtained with an inert tracer. Compartmental network is built mainly on a geometric analysis of reactor and phases distribution. Turbulence exchanges between compartments are derived from turbulence flow fields. The number of compartments varies from 4000 to 18000. (Nauha and Alopaeus, 2015) have studied a bubble column photobioreactor in order to study algae growth. Flow field and light availability are taken into account. The study focuses on a phenomenological model which can be implemented. The bubble size distribution, bubble coalescence and breakup, drag force, light intensity, and zenith angle or length of day are taken into account.

Compartmental Methodology

A rapid overview of the existing papers shows that the rules to set-up the network strongly vary from one situation to another. The proposed method is based on generalizing and establishing rules for the division. If possible, symmetrical and geometrical analysis of the reactor are performed in order to divide the reactor into several slices of similar apparent behavior. Inside each slice, a compartmental network will be defined by compilation and integration of CFD flow simulations, including the most preponderant parameters (for instance flow velocities, turbulence, gas fraction, temperature…). Number of slices is adjusted by fitting RTD curves based on compartmental model with the experimental ones. The analysis of the time constants of the preponderant processes (hydrodynamics, heat/mass transfer and/or chemical reaction) allows to refine locally the network. Exchanges between compartments are based both on convective fluxes (deduced from velocity field) but also on the turbulence exchanges. The full paper will present in detail the methodology and justify its quasi-universality by applying it to several examples of the literature.

Conclusions

A general method for compartmental modeling of chemical reactors is proposed using CFD simulations, tracer experiments and time constant analysis of elementary processes. The quasi-universality of the model is shown by applying it to existing examples from literature.

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